Outflow of Gas Mixtures into Vacuum through a Short Slot

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Abstract. The study of the outflow of binary mixtures into vacuum through a short plane slot was carried out by DSMC method.

FORMULATION OF THE PROBLEM

The outflow of gas mixtures into vacuum through short channels in the transition regime from free molecular to continuum flow is distinct from pure gas flows, which are thoroughly studied for a few decades [1]. As an example, for binary mixtures of monatomic gases one should take into account the availability of three relaxation times. Besides, the inevitable influence of longitudinal parameter gradients gives the variation of a mixture composition along the channel. The probability of molecules escaping of some specie depends on many parameters: the Knudsen number, molecular mass ratio, molecular collision characteristics, accommodation coefficients, and geometry of the channel. In spite of the practical importance of the problem, the outflow of gas mixtures through short channels has not studied well. The results of investigations of flows in the long channel at small pressure gradients are failed for analysis processes in the short channel.

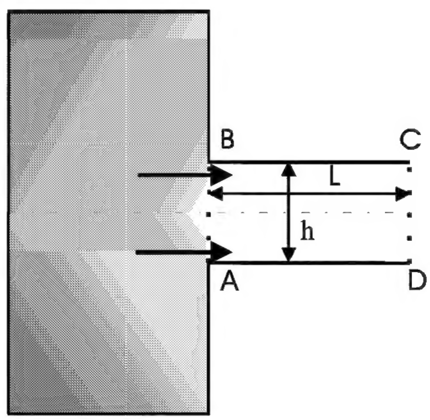

FIGURE 1. General geometry.

The results presented in this paper are obtained by the computational modeling of the steady outflow of binary mixtures into vacuum through a short (up to 100 calibers) plane slot. The physical problem statement is the following one (fig. 1): the gas mixture flows into the infinite slot through the surface AB. The slot length is L, its width is h. It is supposed that the molecules sticking on the surface CD are fully absorbed. The models of the specular and diffuse reflection were used for specification of molecule-surface interaction. The stagnation conditions are predetermined by temperature T_0 and number density of species $n_0 = n_1 + n_2$. The channel wall temperature is taken equal to the stagnation one. The flow of uniform gases is determined by following parameters:

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14. ABSTRACT
The study of the outflow of binary mixtures into vacuum through a short plane slot was carried out by DSMC method.

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1) the Knudsen number $Kn = l / h$, where l is the molecular mean free path in the quiescent gas with stagnation parameters n_0 and T_0;
2) the geometrical parameter L / h;
3) the energy accommodation coefficient α by gas-wall interaction;

The determination of the flows of binary mixtures needs three additional parameters:

1) the species molecular mass ratio m_1 / m_2;
2) mixture composition n_1 / n_2 at the stagnation conditions;
3) collision cross sections of molecules or collision interaction potential parameters.

In this connection the question of definition of flow regimes by the Knudsen number arises. For binary mixtures with the components 1 and 2 it is necessary to take into account three mean free paths between collisions 1-1, 2-2, 1-2.

To date, when not much is known about the low density flows of gas mixtures through short channels, essential simplification of the formulation of the problem is justified. In what follows the consideration will be limited only by one value of stagnation mole fractions $n_1 = n_2$ and one pair of molecular masses $m_1 = 32$ and $m_2 = 16$. The collision parameters of gases, corresponding to their masses, are taken, respectively, for oxygen and methane by determination of VHS and VSS models of molecules accordingly to [2]. The molecules are assumed to be unstructured particles. This assumption is justified for a low pressure by conditions of flow close to isothermal. The Knudsen number is determined by mean free path of oxygen molecules between their collisions.

The problem is solved in two formulations of boundary conditions.

1. It is suggested that the gas mixture of molecules on the left of surface AB (fig. 1) effuses through this surface in the slot with specific flow $n_1 v_1 / 4$ and $n_2 v_2 / 4$, where velocity v_1 and v_2 are the average thermal velocities of molecules at temperature T_0. The molecules returning to the surface AB are fully absorbed. It is equivalent to the boundary condition of evaporation accepted in [3]. It has been shown in [3] that free expansion of the gas into vacuum through the outlet cross section has negligible influence on the flow in the channel. So the given formulation is equivalent to assumption of the full absorption of molecules on the surface CD.
2. The computational modeling embraces the channel and some field (volume) of the gas to the left of the surface AB. The boundaries of this field are chosen at the distance in a few tens of mean free path just to provide negligible effect of a boundary location on the flow in the channel. The natural condition for these boundaries in the frames of the formulated problem is conservation of molar flows of gases at stagnation parameters. This more correct statement of the problem demands much more computational cost.

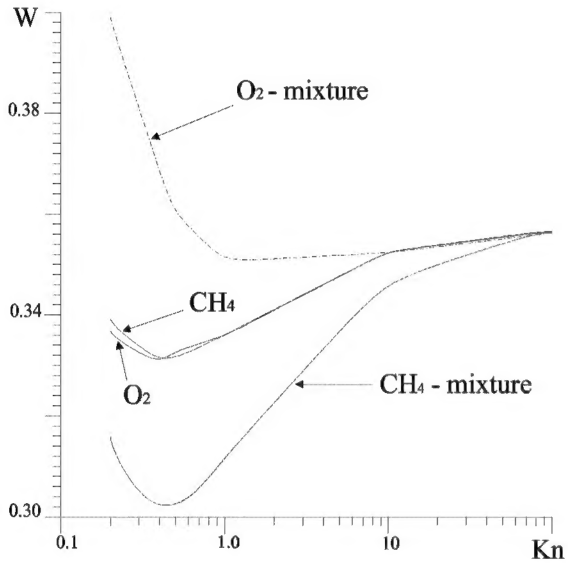
For the solution of the formulated problem the direct simulation Monte Carlo method [2] was used. The intermolecular collisions were specified by the VHS model of molecules [2]. Computations of processes with the VSS model have given almost identical results, not worth of analysis. During the computations density, temperature and velocity of each molecular components were determined. The most attention is focused on analysis of the probability of escaping of molecules into vacuum

$$W = N_e / N_i .$$

Here N_e is the number of molecules escaping out of the slot through the surface CD, and N_i is the number of molecules effused in the same time into the channel through the surface AB at the stagnation parameters. The value W defines the discharge and separation coefficients, that are of great interest for practice. In applied gas dynamics the value of a discharge coefficient for the nozzle is used as ratio of the real gas flux to the flux through the minimum cross section of a nozzle or a channel with isoentropical expansion. The referenced specific flux for the case of expansion into vacuum is obviously equal to product $n^* v^*$, where n^* is number density and v^* is velocity at the Mach number $M = 1$. The discharge coefficient can be determined as probability of escaping of molecules multiplied by value $(n_0 v_0 / 4)/(n^* v^*)$, where $v_0 = \sqrt{8kT_0 / (\pi m)}$. In our case for monatomic gas $(n_0 v_0 / 4)/(n^* v^*)$ =0.546.

RESULTS AND DISCUSSIONS

The investigation was carried out in a wide range of determining parameters: $0.1 \le Kn \le 100$; $3 \le L/h \le 80$; $0 \le \alpha \le 1$; $m_1/m_2 = 2$. On the base of the study of relaxation processes in the expanding gas mixture with different laws of interaction of molecules with channel walls the characteristics of gas discharge through the short channel were determined. Fig.2 shows the dependence of W on the Knudsen number for the mixture of gases $O_2(m_1 = 32)$, $CH_4(m_2 = 16)$ and for separate (pure) gases at L/h=5. The case of diffuse reflection from the wall is considered. Nonmonotonous dependence of W on the Knudsen number is explained by an evolution of relaxation processes from collisionless to continuum flow. By decreasing Kn from infinity the value W drops because of the drag of gas flow by collisions, and then the value W increases because of formation of continuum flow. This behavior of the flow is known as Knudsen paradox, which takes place for gas mixtures as well as for pure gases. As one can see from fig.2 it is more pronounced for the light gas in a mixture. The light gas effectively brakes on the heavy one in regimes of first collision ($Kn \approx 1$). At $Kn \ge 10$ the probability of molecule escaping for mixtures tends to that for pure gases and slightly depends on the Knudsen number. One can consider the flow in the plane slot as free-molecular one at $Kn \ge 10$.



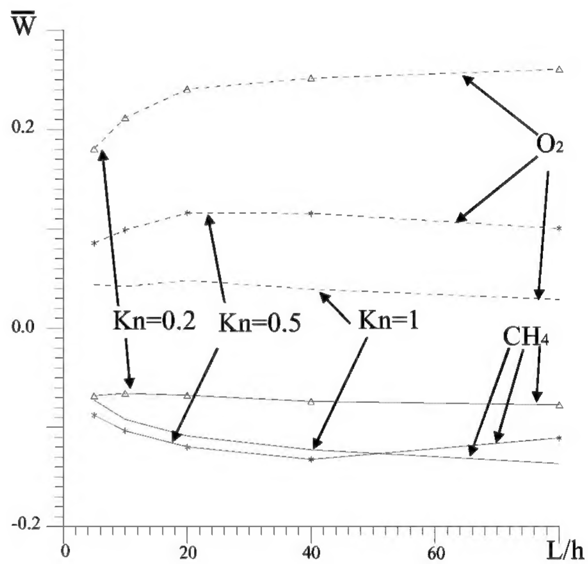


Figure 2. **Figure 3.**

FIGURE 2. The dependence of W on the Knudsen number for the mixture of gases O_2 and CH_4 and for separate (pure) gases.

FIGURE 3. The relative probability $\overline{W}$.

The relative probability of escaping of molecules $\overline{W} = (W_i - W_{im})/W_i$ is presented in fig. 3 as dependence on channel length L/h.

Here W_i and W_{im} are the probabilities of escaping of i-species in the flow of pure gas and mixture. The stabilization of $\overline{W}$ by the slot length increasing (fig.3) and more strong influence of Kn on the heavy molecule escape probability are worth noting as interesting results.

Fig. 4 shows the dependence of W on Kn for the gas mixture flow and flow of the separate components for the specular reflection from the wall ($\alpha = 0$) at $L/h = 5$. The presented data give evidence of the governing influence of the molecular-wall interaction law on the probability of escaping. The Knudsen paradox as effect connected with gas friction on the walls is not pronounced for gas mixture as well as for pure gas. One can observe

the effect, connected with boundary conditions, when number fluxes of "evaporation" of different gases from the surface AB are the same. The probability of escaping of heavy molecules is higher than that of light ones.
This tendency at formulated boundary conditions will be kept for $Kn \to 0$. The flow of a pure gas at $Kn \to 0$ the fraction of molecules returning to the surface of evaporation (effusion) has some asymptotic value. The value 1-W in fig.4 is close to that, obtained for the evaporation from cylinder at $Kn \approx 0.0001$ [4].

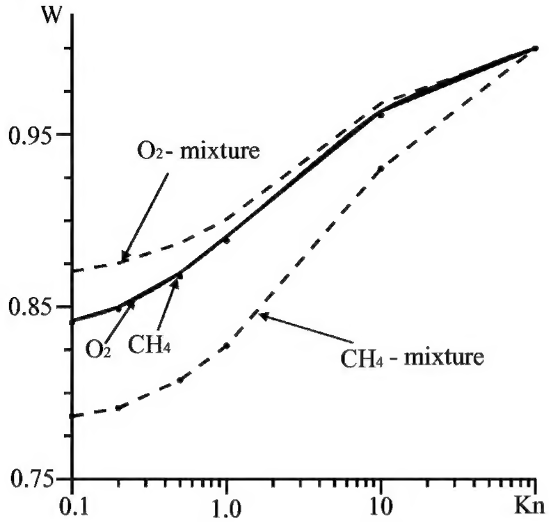


Figure 4.

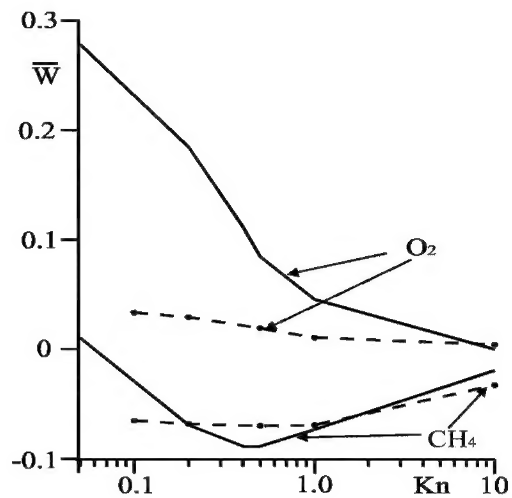


Figure 5.

FIGURE 4. The dependence of W on the Knudsen number for the mixture of gases O_2 and CH_4 and for separate (pure) gases for specular reflection.

FIGURE 5. The dependence of the relative probability $\overline{W}$ on the Knudsen number for diffuse (solid line) and specular (dashed line) reflection.

The relative probability of molecule species escaping for the cases of diffuse and specular reflection in dependence on the Knudsen number is given in fig.5. It is worth to stress the weak effect of Kn on W at specular reflection.

The second formulation of the problem, including the added volume into consideration, refines the gas inlet conditions into the slot because of taking into account the gas expansion before the inlet into slot. Fig. 6 shows the probabilities W for $L/h = 5$. The comparison of data in fig.2 and 6 leads to the conclusion that outflow from the "evaporating" surface and from the added volume is qualitatively the same. But value of W at the transition Knudsen number with essential influence of collisions is higher in the case of expansion from the added volume. It is more pronounced for oxygen as for the gas with more heavy molecules. The Knudsen paradox for the light gas in mixture and for the pure light gas is weaker.

It is obvious that the role of the added volume decreases with increasing the relative slot length *L/h*. The calculations show that at $L/h \geq 30$ the values of W in both formulations are equalizing. This conclusion is quantitatively valid for the given mass and partial density ratios. But one can express the recommendation with a caution that for short channel (in our case $L/h \leq 30$) the calculation of W must be performed with taking into account the added volume.

The role of the added volume takes a generalized form through the relative probabilities. $\overline{W}$ is expressed by the dependence of *L/h* for $Kn = 0.2$ and 1 (fig. 7). The influence of the slot length is rather weak, and influence of the Knudsen number is considerable.

The consideration of the gas separation is beyond the scope of this work. But some general marks are worth to be noted. The obvious result is validation that collision process lowers gas separation to the value below free-molecular one. The separation in the case of the added volume is lower than separation in the case of effusion from the surface AB. By the separation the resting gas is enriched by the heavy component.

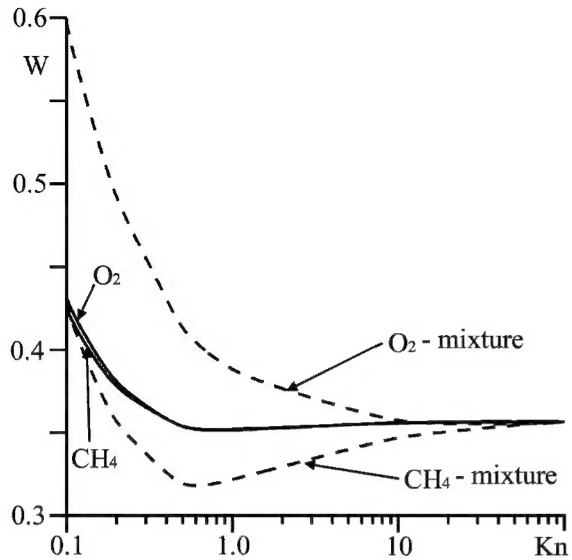


Figure 6.

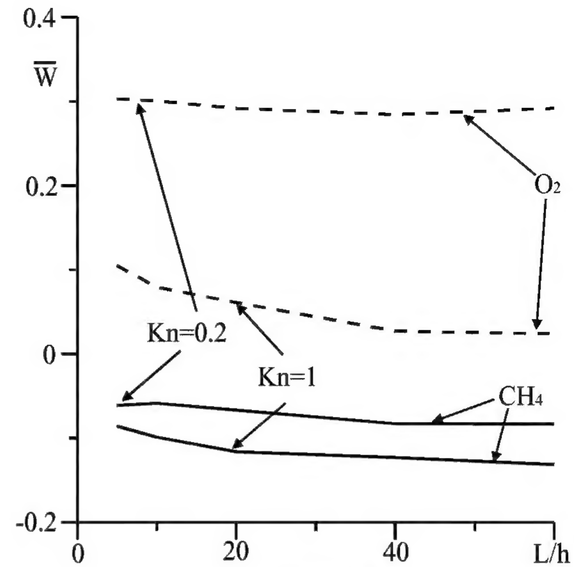


Figure 7.

FIGURE 6. The dependence of W on the Knudsen number for the mixture of gases O_2 and CH_4 and for separate (pure) gases in case of the added volume for L/h=5.

FIGURE 7. The dependence of relative probability $\overline{W}$ on the relative length of channel in case of the added volume for Kn=1 and Kn=0.2.

CONCLUSION

The computational modeling of the outflow of a binary mixture of gases with disparate molecular masses and disparate cross sections through the short plane slot by the DSMC method has elucidated some questions of approaches to the solution the general problem:

- The reason of failure of using the data for long channel for consideration of flows in short channel is clear from presented results.
- The flow can be considered as free-molecular one at $Kn \geq 10$, when outflow is practically independent on inlet boundaries.
- The flow is weakly acted upon inlet boundary conditions of the relative length at $L/h \geq 30$.
- The Knudsen paradox by mixture flow is more pronounced for a light component.
- The relative probabilities of escaping of molecules, depending on the Knudsen number, have weak dependence on the relative length for the case of outflow from the added volume.

The obtained quantitative data are of interest for the conditions embraced in this work. The generalized description of the flows in short channels in transition regimes is not imagined to be realized even for binary mixture. The reason of this is the necessity of taking into account a large number of dissimilar determining criteria. The relatively simple algorithm of DSMC computation open wide possibilities of solving the practical problems in the most sophisticated formulations.

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